Proton structure through large-scale simulations



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Outline

***Introduction & status of lattice Quantum Chromodynamics (QCD)** simulations

- *** 3D structure of the nucleon**
 - Mellin moments
 - ➡ Charges
 - ➡ Form factors
 - ➡Spin content of the nucleon
 - Direct computation of parton distributions

***Conclusions**

*****QCD: gauge theory of the strong interaction

*Lagrangian: formulated in terms of quarks and gluons

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}_{\mu\nu} F^{a\,\mu\nu} + \sum_{f=u,d,s,c,b,t} \bar{\psi}_{f} (i\gamma^{\mu}D_{\mu} - m_{f}) \psi_{f} \qquad D_{\mu} = \partial_{\mu} - ig\frac{\lambda^{a}}{2} A^{a}_{\mu}$$



Harald Fritzsch



Murray Gell-Mann



Heinrich Leutwyler

Phys. Lett. 47B (1973) 365

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#QCD-Gauge theory of the strong interaction #Lagrangian: formulated in terms of quarks and gluons

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*This "simple" Lagrangian produces the amazingly rich structure of strongly interacting matter both at the subatomic level and at large scale in the universe

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}_{\mu\nu} F^{a\,\mu\nu} + \sum_{f=u,d,s,c,b,t} \bar{\psi}_{f} \left(i\gamma^{\mu} D_{\mu} - m_{f} \right) \psi_{f}$$

- *****Unique properties:
 - ★ Confinement
 - ★Asymptotic freedom

David Gross

Frank Wilczek

David Politzer

Nobel prize in Physics 2004

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}_{\mu\nu} F^{a\,\mu\nu} + \sum_{f=u,d,s,c,b,t} \bar{\psi}_{f} \left(i\gamma^{\mu} D_{\mu} - m_{f} \right) \psi_{f}$$

*****Unique properties:

- ★ Confinement
- ★Asymptotic freedom
- \star Mass generation via interaction

Lattice QCD provides an *ab initio* method to study a wide class of strong interaction phenomena

* Lattice QCD uses directly \mathcal{L}_{QCD} or the action $S_{QCD} = \int d^4x \mathcal{L}_{QCD}$

Lattice QCD

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^{a}_{\mu\nu} F^{a\,\mu\nu} + \sum_{f=u,d,s,c,b,t} \bar{\psi}_f \left(i\gamma^{\mu} D_{\mu} - m_f \right) \psi_f$$

• Formulate in path integrals:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[A] \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] \mathcal{O}(\bar{\psi}, \psi, A) e^{i(S_g[A] + S_f[A, \bar{\psi}, \psi])}$$

• Integrate out fermions:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[A] \mathcal{O}(D_f^{-1}[A], A) \left(\prod_{f=u,d,s,c,b,t} \operatorname{Det}(D_f[A]) \right) e^{iS_g[A]}$$

*Discretisation of QCD on a 4-D space-time lattice —> provides a non-perturbative regularisation

- Quark fields on sites: $\psi(x)$ b and t quarks too heavy to include
- Gauge fields on links ~ parallel transporters:

$$U_{\mu}(x) = e^{iagA_{\mu}}$$

Ken Wilson 1974

Lattice QCD

*Discretisation of QCD on a 4-D space-time lattice

- provides a non-perturbative regularisation

- preserves gauge invariance

Mike Creutz 1980

1. Simulation of gauge ensembles {U}:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O}(D_f^{-1}[U], U) \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$
 Rotate to imaginary time
$$P[U] = \frac{1}{Z} \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O}(D_f^{-1}[U], U) \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$

1. Simulation of gauge ensembles {U}: Using HMC

$$P[U] = \frac{1}{Z} \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$

Estimated cost to generate 1000 independent fermion configurations

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Estimated cost to generate 1000 independent fermion configurations

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Many algorithmic improvements:
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1.

2. Domain decomposition 2004, M. Lüscher

3. ...

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \mathcal{O}(D_f^{-1}[U], U) \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$

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1. Simulation of gauge ensembles {U}:

$$P[U] = \frac{1}{Z} \left(\prod_{f=u,d,s,c} \operatorname{Det}(D_f[U]) \right) e^{-S_g[U]}$$

2. Quark propagators or inverse of Dirac matrix D_f[U]: Multi-grid solvers

Linear system to be solved:

$$D_f[U,\mu]v = b$$

Use an adaptive aggregation-based domain decomposition multi-grid approach

A. Frommer, et al., SIAM J.Sci.Comput. 36 (2014) 4, A1581

ETMC: C. A. et al. Phys.Rev.D 94 (2016) 11, 114509, arXiv:1610.02370

Low-lying hadron spectrum

*****BMW collaboration determined the low-lying hadron masses

S. Durr et al., Science 322 (2008) 1224

Low-lying hadron spectrum

*****BMW collaboration determined the low-lying hadron masses, S. Durr *et al.*, Science 322 (2008) 1224
 as well as the mass splittings
 Sz. Borsanyi *et al.*, Science 347 (2015) 1452

	mass splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta\Sigma=\Sigma^\Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta \Xi = \Xi^ \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^{\pm} - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta \Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^{+}$	2.16(11)(17)	-2.53(11)(06)	4.69(10)(17)
$\Delta_{\rm CG} = \Delta N - \Delta \Sigma + \Delta \Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

1. Lattice QCD reproduces the low-lying hadron masses and mass splittings

3D structure of the nucleon

3D structure of the nucleon

*The 3D-structure of the nucleon is a major goal of on-going experiments and the future EIC

*Lattice QCD can contribute towards this goal - many recent developments to compute Mellin moments but also directly parton distributions

Wigner distributions

Longitudinal momentum

 $k^+ = xP^+$

PDF

 $\rho(x, k_T, b_T)$

5-D correlations

Transverse momentum

skewness

PDpartons

TMD

Transverse position

Proton spin puzzle

Spin of all Quarks

*****Proton is made of 3 quarks (valence) of spin 1/2 adding to give total spin of $\frac{1}{2}$ =

- *Deep inelastic scattering experiments with a polarised proton target first by the European Muon Collaboration (EMC) at CERN in 1988 and followup experiments at SLAC and DESY found that only a small fraction of the proton spin is due to the valence quarks —> proton spin puzzle
- ***** The axial charge of the proton measures the intrinsic spin of quarks in the proton $\Delta \Sigma_{q^+} = g_A^q$
- ***** The isovector (u-d) axial charge is accurately known from neutron beta decay

Nuclear transmutation

Proton spin puzzle

*****Proton is made of 3 quarks (valence) of spin adding to give the proton a total spin of $\frac{1}{2}$

*Deep inelastic scattering experiments with a polarised proton target first by the European Muon Collaboration (EMC) at CERN in 1988 and followup experiments at SLAC and DESY found that only a small fraction of the proton spin (25%) is due to the valence quarks —> proton spin puzzle

***** The axial charge of the proton measures the spin of quarks in the proton $\Delta \Sigma_{q^+} = g_A^q$

*Can be compute from the proton matrix element of the axial-vector current

* The isovector axial charge is accurately known from neutron double beta decay

*Easier to compute in lattice QCD since only the connected contribution is needed

Proton isovector axial charge

Lattice QCD results on g_A consistent with experimental value

 $\langle N | \bar{q} \Gamma^{\mu\nu} \tau^3 q | N \rangle$, $\Gamma^{\mu\nu} = \gamma^{\mu}$, $\gamma^{\mu} \gamma_5$, $\frac{1}{2} [\gamma^{\mu}, \gamma^{\nu}]$ • $g_{\rm N} = 1$ • $g_{\rm N} = 1$ • $g_{\rm N} = 1.2723 \pm 0.0023$ (c) reproduce • $g_{\rm T} = 0.53 \pm 0.25$ M. Radici and A. Bacchetta. PRL 120 (2018) 192001

Axial charge

• Axial charges extracted directly from the forward matrix element

Isovector

• Non-zero strangeness, upper limit on charmness of 0.013

• $\sum g_A^q = 0.382(70) \longrightarrow$ intrinsic spin carried by valence quarks: q=u,d,s,c

$$\frac{1}{2}\sum_{q}\Delta\Sigma_{q} = 0.191(35)$$

Isoscalar including disconnected

Proton momentum and spin decomposition

***** Quark unpolarised moment: $\mathcal{O}^{\mu\nu,q} = \bar{q}\gamma^{\{\mu}iD^{\nu\}}q$

 $\langle N(p',s')|\mathcal{O}^{\mu\nu,q}|N(p,s)\rangle = \bar{u}_N(p',s') \Big[A_{20}^q(q^2) \gamma^{\{\mu P^\nu\}} + B_{20}^q(q^2) \frac{i\sigma^{\{\mu\alpha}q_\alpha P^{\nu\}}}{2m} + C_{20}^q(q^2) \frac{q^{\{\mu}q^{\nu\}}}{m} \Big] u_N(p,s)$ Momentum fraction carried $\langle x \rangle_q = A_{20}^q(0)$ $J_q = \frac{1}{2} \left[A_{20}^q(0) + B_{20}^q(0) \right]$ $\mathcal{O}^{\mu
u}$ $(\vec{x}_{\mathrm{ins}}, t_{\mathrm{ins}})$ by a quark $\bigcup_{(\vec{x}_{\rm ins},t_{\rm ins})} \mathcal{O}^{\mu\nu}$ $(\vec{x}_{\rm s}, t_{\rm s})$ (\vec{x}_0, t_0) $(\vec{x}_{\rm s}, t_{\rm s})$ $(\vec{x_0}, t_0)$ * Gluon unpolarised moment lead to an equivalent expression $\mathcal{O}^{\mu\nu,g} = F^{\{\mu\rho}F_{\rho}^{\nu\}}$ $\langle x \rangle_g = A_{20}^g(0) \qquad J_g = \frac{1}{2} \left[A_{20}^g(0) + B_{20}^g(0) \right]$ Field strength tensor Momentum sum: $\sum_{q} \langle x \rangle_q + \langle x \rangle_g = 1$

Intrinsic spin of quarks and momentum sum

Axial charge determines intrinsic spin carried by each quark

Spin sum

***** Spin sum:
$$\sum_{q} J_q + J_g = 0.48(7)$$

2. Nucleon spin sum verified - lattice QCD solves a 30 year puzzle

C. A. *et al.* (ETMC) Phys. Rev. Lett. **119**, 142002, 1909.00485 C. A. *et al.* (ETMC) Phys.Rev.D **101** (2020) 9, 094513, 2003.08486

Proton charge radius puzzle

*****Using muonic hydrogen the proton radius was found to be smaller than what expected R. Pohl et al., Nature 466 (2010) 213

Proton charge radius puzzle

*Using muonic hydrogen the radius was found to be smaller than what expected —> led to many theoretical and experimental investigations

Electromagnetic form factors

*****Proton matrix element of the vector current

Electromagnetic form factors

*****Proton matrix element of the vector current

$$\langle \mathbf{N}(\mathbf{p}', \mathbf{s}') | \mathbf{j}_{\mu} | \mathbf{N}(\mathbf{p}, \mathbf{s}) \rangle = \bar{\mathbf{u}}_{\mathbf{N}}(\mathbf{p}', \mathbf{s}') \begin{bmatrix} \gamma_{\mu} F_{1}(\mathbf{q}^{2}) + \frac{\mathbf{i}\sigma_{\mu\nu} \mathbf{q}^{\nu}}{2m_{\mathbf{N}}} F_{2}(\mathbf{q}^{2}) \end{bmatrix} \gamma_{5} \mathbf{u}_{\mathbf{N}}(\mathbf{p}, \mathbf{s})$$

Dirac Dirac

$$G_{E}(Q^{2}) = F_{1}(Q^{2}) + \frac{Q^{2}}{4m_{N}^{2}}F_{2}(Q^{2}), \quad G_{M}(Q^{2}) = F_{1}(Q^{2}) + F_{2}(Q^{2}), \quad Q^{2} = -q^{2}$$
$$\langle r^{2} \rangle_{E,M} = -\frac{6}{G_{E,M}(0)} \frac{\partial G_{E,M}(Q^{2})}{\partial Q^{2}}|_{Q^{2} \to 0}$$

*Analysis of 6 CLS ensembles with 4 lattice spacings ranging fro, 0.050 fm to 0.086 fm and pion masses ranging from 300 MeV to physical

D. Djukanovic et al. (Mainz), Phys. Rev. Lett. 132 (2024) 21, arXiv:2309.07491; Phys. Rev. D 109 (2024) 9, arXiv:2309.06590

Electromagnetic form factors

D. Djukanovic *et al.* (Mainz), Phys. Rev. Lett. 132 (2024) 21,arXiv:2309.07491; Phys. Rev. D 109 (2024) 9, arXiv:2309.06590 31

Strangeness of the nucleon

Sea quark effects can be accurately determined for EM form factors —> provide precise input to experiments

B-ensemble: $64^3 \ge 128$, a~0.08 fm

Recent results on G_A(Q^2) and G_P(Q^2)

3. Lattice QCD reaches unprecedented accuracy in the evaluation of nucleon form factors

Generalised parton distributions (GPDs)

EIC white paper, arXiv:1212.1701

Direct computation of parton distributions

• PDFs light-cone correlation matrix elements - cannot be computed on a Euclidean lattice z^{-}

$$F_{\Gamma}(x) = \frac{1}{2} \int \frac{dz^{-}}{2\pi} e^{ixP^{+}z^{-}} \langle N(p) | \bar{\psi}(-z/2) \Gamma W(-z/2, z/2) \psi(z/2) | N(p) \rangle |_{z^{+}=0, \vec{z}=0}$$

- Define spatial correlators e.g. along z³ and boost nucleon state to large momentum
 X. Ji, Phys. Rev. Lett. 110 (2013) 262002, arXiv:1305.1539
- Match to the infinite momentum frame using the matching kernel computed in perturbation theory (large momentum effective theory LaMET)

 $z^0 = t$

 z^+

 z^3

Computation of quasi-PDFs

• Compute space-like matrix elements for boosted nucleon states and take the large boost limit

$$\tilde{F}_{\Gamma}(x, P_3, \mu) = 2P_3 \int_{-\infty}^{\infty} \frac{dz}{4\pi} e^{-ixP_3 z} \langle P_3 | \overline{\psi}(0) \Gamma W(0, z) \psi(z) | P_3 / \mu \qquad \text{Renormalise non-perturbatively, } \mathcal{Z}_{(z,\mu)}$$
Need to eliminate both UV and exponential divergences

• Match using LaMET

Perturbative kernel

$$\tilde{F}_{\Gamma}(x,P_3,\mu) = \int_{-1}^{1} \frac{dy}{|y|} C\left(\frac{x}{y},\frac{\mu}{yP_3}\right) F_{\Gamma}(y,\mu) + \mathcal{O}\left(\frac{m_N^2}{P_3^2},\frac{\Lambda_{\text{QCD}}^2}{P_3^2}\right)$$

X. Ji, Phys. Rev. Lett. 110 (2013) 262002, arXiv:1305.1539

C.A. et al. (ETMC) Phys. Rev. Lett. 121, 112001 (2018)

4. Parton distribution functions can be computed directly in lattice QCD

Helicity distributions

$32^3 \times 64$	a=0.0938(3)(2) fm	$m_N = 1.050(8) \text{ GeV}$
L = 3.0 fm	$m_{\pi} \approx 260 \mathrm{MeV}$	$m_{\pi}L \approx 4.0$

C. A., M. Constantinou, K. Jansen, F. Manigrasso, Phys. Rev. Lett. 126 (2021) 10, 102003, arXiv:2009.1306
C.A., G. Iannelli, K. Jansen, F. Manigrasso, Phys. Rev. D 102 (2020) 9, 094508, arXiv:2007.13800

Unpolarized gluon PDF

*Calculate the matrix elements of a spin-averaged nucleon for two gluon fields connected by a Wilson line *Use Wilson flow to reduce ultraviolet fluctuations *Pseudo-PDF approach with pion mass 358 MeV

T. Khan, *et al.* (HadStruc Collaboration) Phys. Rev. D 101 (2021) 094516, 2107.08960 J. Delmar et al. (ETMC) PoS LATTICE2022 (2023) 099, 2212.11399

Generalised parton distributions

*Compute space-like matrix element with different initial and final nucleon boosts in the Breit frame

$$h_{\Gamma}(z,\tilde{\xi},Q^2,P_3) = \langle N(P_3\hat{e}_z + \vec{Q}/2) | \overline{\psi}(z) \, \Gamma W(z,0) \, \psi(0) | \, N(P_3\hat{e}_z - \vec{Q}/2) \rangle$$

$$\tilde{\xi} = -\frac{Q_3}{2P_3} : \text{quasi-skewness} \quad \tilde{\xi} = \xi + \mathcal{O}(\frac{1}{P_3^2})$$

* Rest of the steps are the same as for quasi-PDFs: i.e. renormalise, take the Fourier transform and match and final nucleon boosts

$$\tilde{F}_{\Gamma}(z,\tilde{\xi},Q^{2},P_{3},\mu^{0},\mu_{3}^{0}) = \int_{-1}^{1} \frac{dy}{y} C_{\Gamma}\left(\frac{x}{y},\frac{\mu}{yP_{3}},\frac{\mu_{3}^{0}}{yP_{3}},\frac{(\mu^{0})^{2}}{(\mu_{3}^{0})^{2}}\right) F_{\Gamma}(y,Q^{2},\xi,\mu) + \mathcal{O}\left(\frac{m^{2}}{P_{3}^{2}},\frac{Q^{2}}{P_{3}^{2}},\frac{\Lambda_{\text{QCD}}^{2}}{x^{2}P_{3}^{2}}\right)$$
RI-scale

Reduces to the matching kernel for $\xi=0$ Does not depend on Q^2

X.Ji *et al.*, Phys.Rev. D92 (2015) 014039
X.Xiong, J-H. Zhang, Phys.Rev. D92 (2015) 054037
Y-S. Liu *et al.*, Phys.Rev. D100 (2019), 034006

* First studies for pion and nucleon GPDs

J.W. Chen, H.W. Lin, J.H. Zhang, Nucl. Phys. B 952, 114940 (2020), 1904.12376
C. A. et al., Phys.Rev.Lett. 125 (2020) 26, 262001, 2008.10573
H.-W. Lin, Phys. Rev. Lett. 127, 182001 (2021), 2008.12474
H.-W. Lin, Phys. Lett. B 824, 136821 (2022), 2112.07519

Helicity & transversity GPDs

C. A. *et al.* (ETMC) Phys. Rev. Lett. 125 (2020) 262001,2008.10573 C.A. *et al.*(ETMC), Phys.Rev.D 105 (2022) 3, 034501, 2108.10789

New developments of expressing GPDs in terms of Lorentz invariant amplitudes allows easier access to a range of momentum transfers in lattice QCD calculations

S. Bhattacharya e*t al.* Phys. Rev. D 106 (2022) 114512, 2209.05373 for unpolarized S. Bhattacharya e*t al.* Phys. Rev. D 109 (2024) 034508, 2310.13114 for helicity

5. GDPs can be computed directly in lattice QCD

Transverse momentum distributions (TMDs)

EIC white paper, arXiv:1212.1701

Towards TMD PDFs in lattice QCD

X. Ji, et al. Phys. Rev. D 99 (2019) 114006, 1801.05930

***** Quasi-TMDs formulated in the LaMET approach

M. A. Ebert, I. W. Stewart, Y. Zhao, Phys.Rev.D 99 (2019) 3, 034505, 1811.00026; JHEP 09 (2019) 037, 1901.03685; JHEP 03 (2020) 099 ,1910.08569

First results obtained for the unpolarised nucleon TMD PDF by the Lattice Parton Collaboration (LPC)

X. Ji et al. (LPC) 2211.02340

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$$f^{\mathrm{TMD}}(x,\vec{b}_T,\mu,\zeta) = H(\frac{\zeta_z}{\mu^2}) e^{-\ln\left(\frac{\zeta_z}{\zeta}\right)K(b_T,\mu)} \tilde{f}(x,\vec{b}_T,\mu,\zeta_z) \sqrt{S_r(b_T,\mu)} + \mathcal{O}\left(\frac{\Lambda_{\mathrm{QCD}}^2}{\zeta_z},\frac{M^2}{(P^z)^2},\frac{1}{b_T^2\zeta_z}\right)$$

perturbative matching kernel Collins-Soper kernel, which is nonperturbative for $q_T \sim 1/b_T \sim \Lambda_{QCD}$

Rapidity independent reduced soft function

*Quasi-TMD PDF is given as
$$\tilde{f}^{\text{TMD}}(x, \vec{b}_T, \mu, \zeta_z) = \int \frac{dz}{2\pi} e^{-iz\zeta_z} \frac{P^z}{E_{\vec{P}}} B_{\Gamma}(z, \vec{b}_T, \mu, P^z)$$

Renormalised beam function obtained from the bare

$$\tilde{B}_{0,\Gamma}(z,\vec{b}_T,L,P^z;1/a) = \langle N(P^z)|\bar{\psi}(z/2,\vec{0}_T)\Gamma\mathcal{W}(z,\vec{b}_T,L\hat{z})q(-z/2,\vec{b}_T)|N(P^z)\rangle$$

$$\mathcal{W}(z, \vec{b}_T, L\hat{z}) = \underbrace{\psi_{\tau z/2}}_{-z/2} \underbrace{\psi_{\tau z/2}}_{L_z} b_T$$

Nucleon unpolarised isovector TMD PDF

***** LPC published the first results modelling the momentum dependence and taking the chiral and continuum limits
Jin-Chen He et al. (LPC) arXiv:2211.02340

#ETMC has preliminary results at one lattice spacing (0.093 fm) and heavier than physical pion mass (350 MeV), renormalised with the ratio scheme

Conclusions

- * Lattice QCD provides precision results on low-lying hadron masses and their splitting including isospin and EM effects
- ***** Nucleon charges and form factors are computed to unprecedented accuracy reproducing known quantities such as the axial charge and EM form factors and providing precise results on e.g. tensor charges and axial form factors
- * The so called proton spin and radius puzzles can be understood from lattice QCD computations
- ***** Direct computation of generalised parton distributions is shown to be feasible as is the transverse momentum distributions which is also underway
- *****Many other results are emerging, such as muon g_{μ} -2, properties of resonances and exotics, charm physics, etc.

